A RAINBOW INVERSE PROBLEM

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A. Blasselle[1], V. Calvez[2] and A. Moussa[3]

Abstract. We consider the radiative transfer equation (RTE) with reflection in a three-dimensional domain, infinite in two dimensions, and prove an existence result. Then, we study the inverse problem of retrieving the optical parameters from boundary measurements, with help of existing results by Choulli and Stefanov. This theoretical analysis is the framework of an attempt to model the color of the skin. For this purpose, a code has been developed to solve the RTE and to study the sensitivity of the measurements made by biophysicists with respect to the physiological parameters responsible for the optical properties of this complex, multi-layered material.

Résumé. On étudie l'équation du transfert radiatif (ETR) dans un domaine tridimensionnel infini dans deux directions, et on prouve un résultat d'existence. On s'intéresse ensuite à la reconstruction des paramètres optiques à partir de mesures faites au bord, en s'appuyant sur des résultats de Choulli et Stefanov. Cette analyse sert de cadre théorique à un travail de modélisation de la couleur de la peau. Dans cette perspective, un code à été fait pour résoudre l'ETR et étudier la sensibilité des mesures effectuées par les biophysiciens par rapport aux paramètres physiologiques tenus pour responsables des propriétés optiques de ce complexe matériau multicouche.

Introduction

Skin is a complex multi-layered media and the most important organ of our body in terms of weight, surface and functionalities. For many years, physicists have tried to understand what physiological components or properties are responsible for its color. The color of an object is defined by a unidimensional curve called the *reflectance spectrum*, which is the relative energy given back by the object for each wavelength of the visible range, when it is enlighted with a white spot. Physicists have developed a lot of models to link the physiological components of the skin (like, for example, the blood concentration or the diameter of the melanosomes) to its optical properties. Physicists have simulated, by many ways, how light travels into the skin. What has not been theoretically investigated yet, even if very well studied by Magnain and Elias in [2], is the inverse problem of retrieving the physiological parameters from measurements made at the surface of the skin.
Before studying the inverse problem, we tried to simulate the direct one, and developed a small Matlab code to do so. This code is proved to be quite satisfying for this purpose, hence we used it to make a sensitivity study of the reflectance curves with respect to the physiological parameters. We went on with the theoretical study of this inverse problem, in a very simplified framework and based on the existing work of Choulli and Stefanov [5]. The paper is organized in the reverse order: theoretical study, then numerical results.

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1. Modeling

1.1. The radiative transfer equation

When light enters an object X, the photons propagate in straight line, unless they are absorbed by the material or scattered (and possibly deviated) by various entities. One classical way to describe the light intensity is the use of a *probability density function* (p.d.f.): f, that depends on the position x and the velocity v of the photon.

The set of all possible directions, V is all or part of the sphere $\mathbb{S}^2$. The physical interaction with the material is described by:

- the absorption coefficient μ_a (given in m^{-1}), which is the number of absorption events per unit length and depend on the position and the direction: $\mu_a = \mu_a(x, v)$
- the scattering coefficient $\mu_s = \mu_s(x, v)$ (also in m^{-1}), the same quantity for the scattering
- the kernel $p = p(x, v, w)$ which is a probability density with respect to v. It denotes the probability for a photon arriving with the direction w, to get a new direction v after having hit a scatterring center.

If the scattering centers are distant enough from one another (compared to the wavelength), the radiative transfer equation (RTE) describes properly the behaviour of the light intensity:

$$v \cdot \nabla_x f + (\mu_a(x, v) + \mu_s(x, v))f(x, v) = \int_V \mu_s(x, w)p(x, v, w)f(x, w) \ \mathrm{d}w \qquad \text{in } X \times V \tag{1}$$

1.2. Geometry and boundary conditions

The equation (1) has been written with no internal source of light, and has to be complemented by boundary conditions to model the enlightment of the object. The typical experiment we are interested in is the following: the skin is enlighted from its top, on a large surface, and its color is registered on the same zone. At this scale, the two others dimensions can be considered as infinite. Indeed, the thickness of the whole skin is of the order of 10^{-3} m, whereas the skin is much more extended over our body. Hence, we will model our skin sample as a box infinite in the two planar directions.

When travelling into the skin, the light will encounter several interfaces, one of them being the epidermis-dermis junction. Part of the light will get through it, but the remaining amount will be reflected. Hence, our boundary conditions will be:

- a source function f_- modeling the enlightment on the top
- reflection of part of the light at each interface encountered.

2. Theoretical inverse problem

Choulli and Stefanov have already proved in [5] that the parameters can be uniquely determined by surface measurements, under the following assumptions, in the case where the RTE (1) is complemented with Dirichlet boundary conditions. We will conduct the same study with mixed boudary conditions by adding a reflection operator. Before getting into the inverse problem, we have to show existence of the light intensity for the direct problem.

2.1. Notations and functional framework

We focus in this study on a single layer, so that the first interface encountered is the bottom of the sample. Hence, the position and velocity spaces are:

$$X =]0, L[\times\mathbb{R}^2, \quad V = \mathbb{S}^2. \tag{2}$$

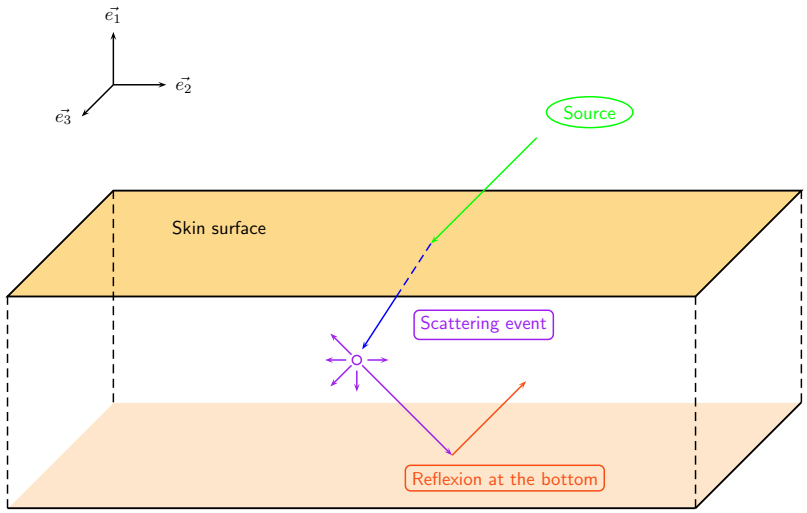

FIGURE 1. Model of the skin

We consider a system of axis on X whose first direction is normal to the plane of the skin, as illustrated in Figure 1.2. All points belonging to the boundary of X (that is $\partial X = \{0\} \times \mathbb{R}^2 \cup \{L\} \times \mathbb{R}^2$) are denoted with a prime symbol: x', y' and so forth. For $x' \in \partial X$, we denote by $n(x')$ the outward-pointing normal vector. The following sets will be widely used:

$$\Gamma^{\pm} = \{\xi = (x', v) \in \partial X \times V / \pm v \cdot n(x') > 0\},$$

with the measure $\mathrm{d}\xi = |v.e_1|\,\mathrm{d}x'\,\mathrm{d}v$. We define the first time of exit by outward (resp. downward) directions:

$$\tau^{\pm}(x, v) = \min\{t \geq 0 | x \pm tv \in \partial X\}, \quad \tau(x, v) = \tau^{-}(x, v) + \tau^{+}(x, v).$$

We also introduce the absorption coefficient, and the full scattering kernel:

$$\sigma_a(x, v) = \mu_a(x, v) + \mu_s(x, v),$$
$$k(x, v, w) = \mu_s(x, w)p(x, v, w).$$

The enlightment is modeled by $f_- \in \mathrm{L}^1(\Gamma^-, \mathrm{d}\xi)$. The coefficients are assumed to satisfy the following regularity properties [6]:

(i) $0 \leq \mu_s \in \mathrm{L}^\infty(X \times V)$ and $0 < \nu \leq \mu_a \in \mathrm{L}^\infty(X \times V)$
(ii) $0 \leq k(x, v, .) \in \mathrm{L}^1(V)$ for a.e. $(x, v) \in X \times V$

The problem will be studied in the following functional space:

$$W = \{f \in \mathrm{L}^1(X \times V) \text{ s.t. } v \cdot \nabla f \in \mathrm{L}^1(X \times V)\}. \tag{3}$$

Thanks to Cessenat [3,4], we know that if $f \in W$, its traces on $\Gamma^{\pm}$ exist and we give the theorem in the case of L^1 spaces:

Theorem 2.1 (Cessenat). *The trace operator $u \mapsto u|_{\Gamma^{\pm}}$ is continuous from W in $\mathrm{L}^1(\Gamma^{\pm}, \mathrm{d}\xi)$*

We denote classically the albedo operator as follows:

$$\mathcal{A}f_- = f|_{\Gamma^+},$$

where $f(x,v)$ satisfies (1) with the boundary condition $f = f_-$ on Γ_-. The Boundary Value Problem admits a unique solution in W if $f_- \in L^1(\Gamma^-, d\xi)$ [6]. Also the albedo operator $\mathcal{A} : L^1(\Gamma^-, d\tilde{\xi}) \to L^1(\Gamma^+, d\tilde{\xi})$ is a bounded operator, where the boundary measure $d\xi$ has been replaced by $d\tilde{\xi} = \min\{\tau(x,v), K\}|v \cdot e_1| \,\mathrm{d}x' \,\mathrm{d}v$ for some positive number K [5].

2.2. **The direct reflection problem**

We define a general reflection operator $\mathcal{R} : \mathrm{L}^1(\Gamma^+, \mathrm{d}\xi) \to \mathrm{L}^1(\Gamma^-, \mathrm{d}\xi)$ by:

$$\mathcal{R}\varphi = \int_{w.n(x')>0} m(x', v, w)\varphi(x', w) \,\mathrm{d}w, \tag{4}$$

where $m(x', v, w)$ is a boundary transition kernel such that $\mathcal{R}$ satisfies the following assumption: there exists $0 \leq \alpha < 1$ such that,

$$\forall \varphi \in \mathrm{L}^1(\Gamma^+, \mathrm{d}\xi) \quad \|\mathcal{R}\varphi\|_{\mathrm{L}^1(\Gamma^-, \mathrm{d}\xi)} \leq \alpha \|\varphi\|_{\mathrm{L}^1(\Gamma^+, \mathrm{d}\xi)} \tag{5}$$

If, under our geometrical framework (plane interfaces), we assume that the skin satisfies Snell-Descartes reflection laws at its interfaces (like in our numerical implementation), some grazing rays may be trapped in the material because of the values of the optical indices if we do not remove the planar directions v (such that $v.e_1 = 0$). Hence, the latter assumption is not satisfied for the corresponding reflection operator. The equation (5) expresses that every direction is uniformly partially absorbed (or refracted). In our code, we removed the grazing directions with the angular discretization.

The direct problem we are interested in writes:

$$\begin{cases} v \cdot \nabla_x f(x,v) + \sigma_a(x,v) f(x,v) = \displaystyle\int_V k(x,v,w) f(x,w) \,\mathrm{d}w & \text{in } X \times V \\ f|_{\Gamma^-} = f_- + \mathcal{R} f|_{\Gamma^-} & \text{on } \Gamma^- \end{cases} \tag{6}$$

Theorem 2.2. *Suppose that $f_- \in \mathrm{L}^1(\Gamma^-, \mathrm{d}\xi)$, the reflection operator $\mathcal{R}$ verifies* (5) *and assumptions* (i) *and* (ii) *hold true. Then the problem* (6) *has a solution f in W.*

Proof. We define the operator $\mathcal{T} : \mathrm{L}^1(\Gamma^-, \mathrm{d}\xi) \to \mathrm{L}^1(\Gamma^-, \mathrm{d}\xi)$:

$$\mathcal{T}g = \mathcal{R} \circ \mathcal{A}g. \tag{7}$$

We know that this system has a unique solution in W. We have that $\mathcal{T}$ is a contraction operator. Assume first that g and f are nonnegative functions. If we integrate (1) on $X \times V$ and use Green formula, we get:

$$\begin{aligned} \int_{\Gamma^+} v \cdot n(x') f|_{\Gamma^+}(x', v) \,\mathrm{d}x' \,\mathrm{d}v + \int_{\Gamma^-} v \cdot n(x') g(x', v) \,\mathrm{d}x' \,\mathrm{d}v + \int_{X \times V} \sigma_a(x,v) f(x,v) dx dv \\ = \int_{X \times V} \int_V k(x,v,w) f(x,w) dx dv dw \\ = \int_{X \times V} \mu_s(x,w) f(x,w) dx dw. \end{aligned}$$

Therefore we have:

$$\int_{\Gamma^+} f|_{\Gamma^+} \,\mathrm{d}\xi - \int_{\Gamma^-} g \,\mathrm{d}\xi = -\int_{X \times V} \mu_a(x,v) f(x,v) dx dv \leq 0.$$

For a function whose sign is unknwon, we begin by multiplying (1) by $\mathrm{sgn}(f)(x,v)$ and then we integrate by parts. Using the fact that $\nabla|f| = \mathrm{sgn}(f)\nabla f$, and $\mathrm{sgn}(f)f = |f|$ we obtain the exact same conclusion for functions having no specific sign, namely that:

$$\|f\|_{\mathrm{L}^1(\Gamma^+,\,\mathrm{d}\xi)} \leq \|g\|_{\mathrm{L}^1(\Gamma^-,\,\mathrm{d}\xi)}.$$

The assumption (5) directly ensures that $\mathcal{T}$ is a contraction operator. Denoting by I the identity of $\mathrm{L}^1(\Gamma^-,\,\mathrm{d}\xi)$, we know that $I-\mathcal{T}$ is invertible. Thereby the solution of (6) satisfies

$$(I-\mathcal{T})f = f_- \qquad \text{on } \Gamma^-. \tag{8}$$

□

2.3. **The inverse problem without reflection**

We assume in this Section that the absorption coefficient σ_a does not depend on the velocity v. In [5], the authors prove that under suitable assumptions, the albedo operator $\mathcal{A} : f_- \to f|_{\Gamma^+}$ determines uniquely the coefficient $\sigma_a(x)$. In addition, when the space dimension is higher than 3, the albedo operator also characterizes the scattering kernel $k(x,v,w)$.

We briefly sketch their arguments below. The main idea is to decompose the albedo operator into three parts: the solution to (1) with the boundary condition $f_- = \delta_{\Gamma^-}(x'-x_0')\delta_V(v-v_0)$ is given by $f(x,v) = f_1(x,v) + f_2(x,v) + f_3(x,v)$, where f_1 is the contribution of an incoming laser subject to absorption only. It verifies:

$$v\cdot\nabla f_1(x,v) + \sigma_a(x)f_1(x,v) = 0, \tag{9}$$

and the solution is explicitely given by:

$$f_1(x,v) = |n(x_0')\cdot v_0| \int_0^{\tau_+(x,v)} \exp\left(-\int_0^{\tau_-(x,v)} \sigma_a(x-pv)\,\mathrm{d}p\right)\delta(x-x_0'-tv)\delta(v-v_0)\,\mathrm{d}t. \tag{10}$$

The second contribution f_2 results from trace of this laser (a single line parametrized by $x_0' + tv_0$) which is scattered and absorbed. It satisfies:

$$v\cdot\nabla_x f_2(x,v) + \sigma_a(x)f_2(x,v) = \alpha(x,v_0)k(x,v,v_0)\delta(x-\tau_-(x,v_0)v_0), \tag{11}$$

and the solution is explicitely given by:

$$\begin{aligned} f_2(x,v) = |n(x_0')\cdot v_0| \int_0^{\tau_-(x,v)} \int_0^{\tau_+(x,v)} \exp\left(-\int_0^{s} \sigma_a(x-pv)\,\mathrm{d}p\right) \\ \times \exp\left(-\int_0^{\tau_-(x-sv,v_0)} \sigma_a(x-sv-pv_0)\,\mathrm{d}p\right) k(x-sv,v_0,v)\delta(x-x_0'-sv-tv_0)\,\mathrm{d}t\,\mathrm{d}s. \end{aligned} \tag{12}$$

The reminder f_3 has no explicit formulation. However it is proven in [5] that it is a function. Namely, it satisfies the following estimate:

$$(\min\{\tau,K\})^{-1}|n(x_0')\cdot v_0|^{-1} f_3(x,v) \in L^1(X\times V) \quad \text{uniformly in } (x_0',v_0). \tag{13}$$

Let us sketch the arguments of [5] in our context (see also [1] for a comprehensive review). We restrict to $x_0' = 0$ for the sake of clarity. At first glance we look for a solution of the form

$$f(x,v) = \alpha(x,v)\delta(x-\tau_-(x,v)v)\delta(v-v_0) + g(x,v), \tag{14}$$

where $g(x,v)$ contains lower order distribution terms (namely either the support of the singular parts is of lower dimension, or they are simply functions [1, 5]). Plugging (14) into (1), we obtain the following equation for α and g:

$$\begin{aligned} v\cdot\left(\nabla_x\alpha(x,v)\delta(x-\tau_-(x,v)v)+\alpha(x,v)\left(\mathrm{Id}-e_1\otimes\frac{v}{v\cdot e_1}\right)\nabla_x\delta(x-\tau_-(x,v)v)\right)\delta(v-v_0)\\ +\sigma_a(x)\alpha(x,v)\delta(x-\tau_-(x,v)v)\delta(v-v_0)+v\cdot\nabla_x g(x,v)+\sigma_a(x)g(x,v)\\ =\alpha(x,v_0)k(x,v,v_0)\delta(x-\tau_-(x,v_0)v_0)+\int_w k(x,v,w)g(x,w)dw, \end{aligned}$$

where we have used the explicit formulation: $\tau_-(x,v)=\dfrac{x\cdot e_1}{v\cdot e_1}$. Therefore we get:

$$\begin{aligned} &\left(v\cdot\nabla_x\alpha(\tau_-(x,v_0)v_0,v_0)+\sigma_a(\tau_-(x,v_0)v_0)\alpha(\tau_-(x,v_0)v_0,v_0)\right)\delta(x-\tau_-(x,v_0)v_0)\delta(v-v_0)\\ &\quad+v\cdot\nabla_x g(x,v)+\sigma_a(x)g(x,v)=\alpha(x,v_0)k(x,v,v_0)\delta(x-\tau_-(x,v_0)v_0)+\int_w k(x,v,w)g(x,w)dw. \end{aligned}\tag{15}$$

By identifying the leading order term (a direct product of Dirac masses), we eventually obtain:

$$v\cdot\nabla_x\alpha(\tau_-(x,v_0)v_0,v_0)+\sigma_a(\tau_-(x,v_0)v_0)\alpha(\tau_-(x,v_0)v_0,v_0)=0,$$

in other words,

$$\frac{d}{ds}\alpha(x(s),v_0)+\sigma_a(x(s))\alpha(x(s),v_0)=0,\quad x(s)=sv,\quad s=0\dots\tau_+(0,v_0).$$

This equation essentially determines the fate of a laser without scattering. The solution is known as the Radon (or X-ray) transform of σ_a:

$$\alpha(x,v)=\exp\left(-\int_0^{\tau_-(x,v)}\sigma_a(x-sv)ds\right).$$

In particular, this entirely determines the absorption rate $\sigma_a(x)$ (cf. [5, 7] and references therein).

The next contribution in the development of $g=f_2+f_3$ is issued from secondary scattering of this first dominant laser trace, namely the transport equation with source term (11), which is solved assuming that the last integral contribution is negligible in (15). The boundary value is $f_2|_{\Gamma_-}=0$. Consequently, one may compute the measure solution of (11). It explicitely writes as follows:

$$f_2(x,v)=\int_{t=0}^{\tau_-(x,v)}\exp\left(-\int_{s=0}^{t}\sigma_a(x-sv)ds\right)\alpha(x-tv,v)k(x-tv,v,v_0)\delta(x-tv-\tau_-(x-tv,v_0)v_0)dt.\tag{16}$$

One of the major conclusion of [5] concerns the role of the dimension. Indeed, if $N\geq 3$ a ray (x,v) in the phase space $X\times V$ will not go through the support of the source $\{x=\tau_-(x,v_0)v_0\}\times\{v_0\}$ except on a zero-measure set. This is not the case in dimension 2. As a consequence, the distribution (16) is a singular measure as soon as $N\geq 3$, because it is supported on rays issued from the laser source. Hence it can be distinguished from the reminder f_3 (13). This enables to retrieve the scattering kernel k. Such a procedure cannot be performed in dimension 2. The stability issue of the inverse problem is discussed in [1].

To conclude this theoretical presentation of the inverse problem, let us mention the generalization of above results to the case of pure reflection (without scattering and refraction at the interface) when measurements are possible only at the upper boundary (from where the laser is issued). First, the dominant contribution is given

by the successive reflection of the laser:

$$f_1(x,v) = \sum_{n\geq 0} \alpha_n(x,v)\delta\left(x - x_n - \tau_-(x,v_{io})v_{io}\right)\delta\left(v - v_{io}\right) + g(x,v),$$

where v_{io} denotes successively the incoming $v_i = v_0$ or the outcoming $v_o = \mathcal{R}v_0$ velocity, and x_n is the sequence of impact points. We focus on $\alpha_1(x_2, v_o)$ which combines successive absorptions along the two first rays:

$$\alpha_1(x,v_o) = \exp\left(-\int_0^{\tau_-(x_1,v_i)} \sigma_a(x_i - sv)ds\right) \times \exp\left(-\int_0^{\tau_-(x_2,v_o)} \sigma_a(x_2 - sv_o)ds\right).$$

It is known that the first term in the product, namely the Radon transform, characterizes the absorption rate σ_a [7]. It would be interesting to prove whether or not the product also characterizes σ_a.

The second contribution f_2 can be expressed as above. It shares similar properties with the case without reflection: namely it is a singular measure in dimension $N \geq 3$. So we expect the Albedo operator to characterize the scattering kernel in the presence of reflection too.

3. Numerical simulations

3.1. **Simplifying assumptions**

We do not focus on a single layer anymore, because skin is structured in many of them. We only consider here the most important ones: the epidermis, the dermis and the hypodermis. We assume that the absorption and scattering coefficients are constant in each part, and that the probability density function obeys the Henvyey-Greenstein law, namely:

$$p(x,v,w) = \frac{1-g^2}{(1+g^2-2gv.w)^{\frac{3}{2}}},$$

where g is the anisotropy factor and is constant in each layer, as described in [8]. The enlightment we want to model presents cylindrical symmetry, so we get rid of the second spherical angle, to keep the angle with respect to the skin plane. Hence, we only need two scalars: one for the depth (the position), and one for the angle (the direction).

To model the Snell-Descartes law at each interface, we assigne the reflection operator as follows: $\mathcal{R}\varphi(x',v) = a(x',v)\varphi(x',\tilde{v})$, where $\tilde{v} = (-v_1, v_2, v_3)$. But as we are now interested in what happens on both sides of the interfaces, we have to consider the refraction too. If we consider one of our interfaces, and denote by n_u, resp. n_d, the optical index of the upward, resp. downward, layer, the refraction operator can be expressed as $\mathcal{F}\varphi(x',v) = b(x',v)\varphi(x',\hat{v})$ where $\hat{v}$ is the direction after refraction given by the well known Snell-Descartes formula $n_u \sin\alpha_u = n_d \sin\alpha_d$, and b is the refraction factor, computed from the optical indices.

Remark 3.1. The factor a which is computed from the optical indices of the inner layers of the skin is equal to 1 for sufficiently grazing directions. Indeed, the optical indices are generically higher in the skin than in the air, hence grazing rays are trapped inside the skin. Therefore the assumption (5) is not satisfied in this framework. However it is not expected that the transfer of photons at the interface between skin layers obeys perfect Snell-Descartes law (diffraction is expected to play a role). As far as numerics are concerned, we use the contractive effect of the absorption part $\mu_a \geq \nu > 0$ to ensure convergence of the scheme.

3.2. **Implementation**

To get the discretization formula, we evaluate (1) in $x - tv$, then multiply by $\exp\left(-\int_0^t \sigma_a \, \mathrm{d}s\right)$ and integrate from $t = 0$ to $t = \Delta t$:

$$f(x,v) = \exp\left(-\int_0^{\Delta t} \sigma_a \, \mathrm{d}s\right) f(x - v\Delta t, v) + \int_0^{\Delta t} \exp\left(-\int_0^t \sigma_a \, \mathrm{d}s\right) A_2 f(x - tv, v) \, \mathrm{d}t.$$

where A_2 is the scattering operator. In this formula, x is implicitely assumed to belong to $\mathbb{R}^3$. In order to adapt it to our unidimensional case, we have to choose properly the step Δx. We opt for $(v.e_1)\Delta t = \Delta x$, where $v.e_1 = \sin(\Delta\theta) > 0$ is the vertical component of the first discrete velocity.

Assuming that the scattering is piecewise constant and writing this formula between two points, we obtain the following discretization formula:

$$f^{n+1}(x + \Delta x, v) = f^{n+1}(x,v) \exp\left(-\frac{\sigma_a \Delta x}{v.e_1}\right) + \frac{1}{\sigma_a}\left(1 - \exp\left(-\frac{\sigma_a \Delta x}{v.e_1}\right)\right) A_2(f^n)(x,v). \tag{17}$$

The inputs are the values of the physiological parameters, and the output of interest is the reflectance spectrum of the corresponding skin (which is the information collected at the outward surface of the skin). Nevertheless, the intensity of the light is computed in the whole tissue. The structure of the code is the following:

- loop over all the wavelengths
- convergence loop, that does not stop until $\|f^{n+1} - f^n\| < \varepsilon$
- loop over all the layers to propagate the light, using (17)
- loop over all the layers to update the boundary conditions at each interface, using Snell-Descartes laws.

For each simulation, we monitor if the total mass is preserved, to ensure that the code do not create or destroy too much energy. For a source of total energy 1, the loss due to the code never exceeds 2%. To obtain the reflectance curve, we integrate, for a given wavelength, the light intensity at the upper surface over all the outgoing directions. This gives the reflectance, denoted by $S(\lambda)$. Then, we compute the so-called *relative reflectance*, $S_r(\lambda)$:

$$S_r(\lambda) = \frac{S(\lambda) - S(380)}{S(780) - S(380)}.$$

3.3. **The direct problem**

Our code has been compared to a reliable Monte-Carlo code that sends directly photons in the material. The following results have been obtained by setting in our code:

- $[100, 100, 20]$ points for, respectively: epidermis, dermis, hypodermis,
- 160 angular samples for the whole sphere,
- 100 wavelengths, from 380 to 780 nm ,
- a tolerance of 10^{-7} for the convergence loop.

and by sending 10000 photons in the Monte-Carlo code.

Remark 3.2. During this validations, we noted that the optical index of the hypodermis is crucial and severely affects both S and S_r.

Our simulation is based on the three main layers, whereas in the Monte-Carlo code, a multiplicative factor is used to take into account the full behaviour from the hypodermis. When a photon arrives at the dermis-hypodermis junction, it is either absorbed or reflected according to a pre-computed law. We show on the figure 2 the most delicate numerical experiment to reproduce. The optical index of the hypodermis has been carefully

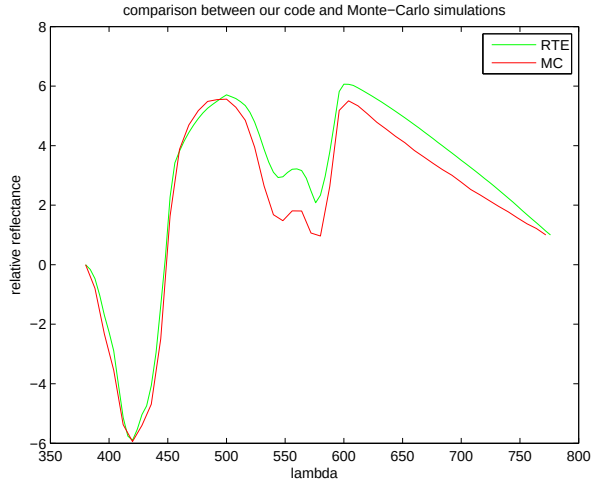

FIGURE 2. Relative reflectances for a given set of physiological parameters

chosen to adjust the relative spectrum in a good agreement. We gain a time factor from 2 up to 3 in the good cases as opposed to the Monte-Carlo code.

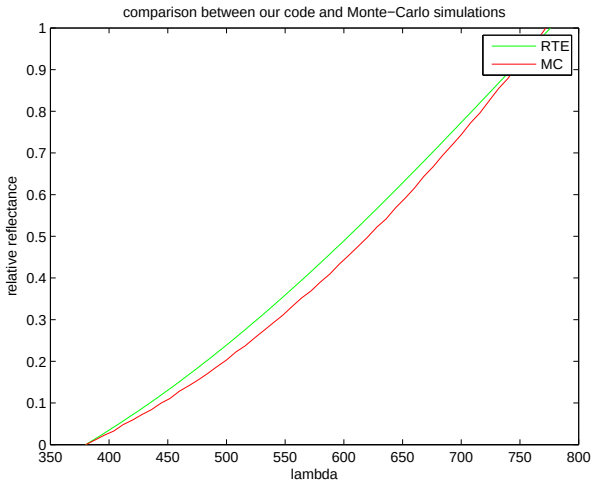

FIGURE 3. Relative reflectances for another set of physiological parameters

The figure 4 is a representation of the light intensity in the whole skin and for all the directions, for the wavelength $\lambda = 456$ nm and for the following values of (μ_a, μ_s) in each layer: epidermis $(1.69, 88.43)$, dermis $(0.985, 260.11)$ and hypodermis $(9.2720, 1186.4)$.

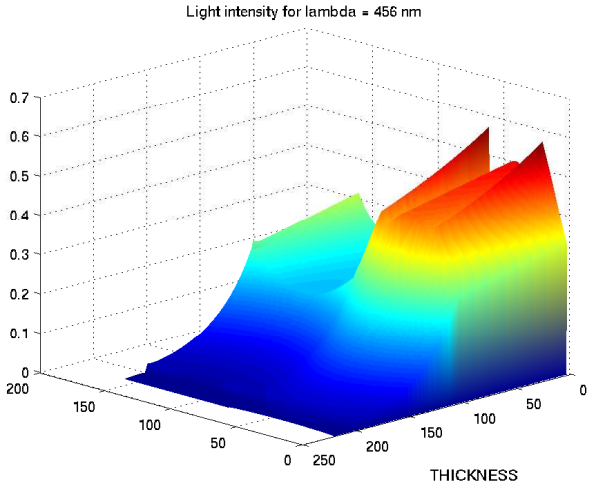

FIGURE 4. Light intensity for $\lambda = 456$ nm

3.4. **Study of the derivatives**

It would be interesting to retrieve the physiological parameters from the reflectance curve. To this end, we observe that the derivative of the intensity with respect to a parameter p_i verifies the exact same transport equation with a given source term:

$$v \cdot \nabla_x \frac{\partial f}{\partial p_l} + \sigma_a \frac{\partial f}{\partial p_l} = \int_{\mathbb{S}^2} k(v,w) \frac{\partial f}{\partial p_l}(x,w,\lambda)\,\mathrm{d}w - \frac{\partial \sigma_a}{\partial p_l} f + \int_{\mathbb{S}^2} \frac{\partial k}{\partial p_l}(v,w) f(x,w,\lambda)\,\mathrm{d}w. \tag{18}$$

Hence the derivatives can be computed very easily from the same code and with the same scheme. So, once we have computed the light intensity, we use it in the source term of (18). From those derivatives, we can compute the derivatives of the reflectance curve with respect to each physiological parameter. On the figure 5, we present the derivatives of the reflectance curve with respect to three physiological parameters. This kind of result can help to understand in which range of wavelengths each component has a relative influence on the color of the skin. For example, looking at the right image, we can deduce that this physiological parameter has an influence on the color on the skin only for the wavelengths belonging to $[450nm; 540nm]$.

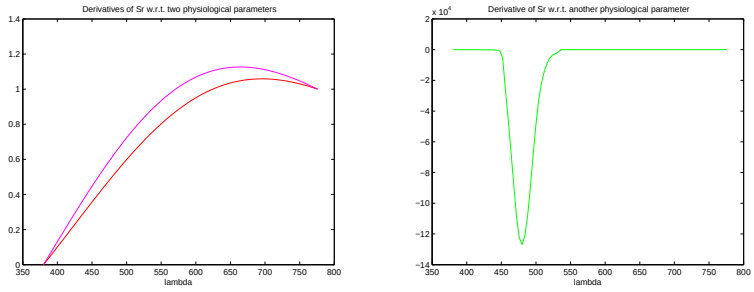

FIGURE 5. Derivatives of $S_r(\lambda)$ w.r.t. various physiological parameters

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